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First-principles study of strain-induced ferromagnetism in $LaCoO_3$ HOSUNG SEO, ALEXANDER DEMKOV, The University of Texas at Austin — We study theoretically the effect of biaxial strain on magnetic properties of $LaCoO_3$ (LCO) using density functional theory combined with the Hubbard U method. LCO is normally a non-magnetic insulator with trivalent cobalt ions in low-spin state (t_{2g}^6). Owing to close interplay between orbital, spin, and lattice degrees of freedom, it shows rich magnetic behavior such as temperature-induced spin state transition. Recently, the ferromagnetic tensile-strained LCO films have been reported. The underlying physics of the ferromagnetic state is, however, unclear. Using a large tetragonal cell we calculate full structural response of the system to applied strain for non-magnetic and magnetic solutions. We show that beyond tensile strain of 3.8% the ferromagnetic solution with Co ions in intermediate-spin state (t_{2g}^5 e_g^1) is stabilized accompanied by partial untilting of CoO_6 octahedral network. We also perform the calculation for compressive-strained structures and the difference between these and the tensile strained structures will be presented.

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